4-Hydroxyphenylacetate
3233-32-7 | DTXSID70186062

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 47.7 L/kg

Global applicability domain: Inside

Local applicability domain index: 7.20e-01

Confidence level: 8.31e-01

Nearest Neighbors from the Training Set

Image not found
N-Methyl-N'-phenylurea
Measured: 19.5
Predicted: 29.8

Image not found
Methyl phenylcarbamate
Measured: 53.7
Predicted: 59.1

Image not found
(2-Chlorophenyl)urea
Measured: 40.7
Predicted: 51.3

Image not found
Methyl N-(3-chlorophenyl)carbamate
Measured: 141
Predicted: 94.1